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Structural and dynamic features of water and amorphous ice

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Abstract

© 2017, Pleiades Publishing, Ltd.Structural properties and microscopic dynamics of water and amorphous ice have been studied by the molecular dynamics method. It has been found that the distribution function of the tetrahedricity parameter exhibits two ranges, which correspond to local molecular formations with low and high degrees of tetrahedricity. The number of molecular clusters with a high degree of tetrahedricity grows as temperature decreases. It has been shown that the vibrational density of states comprises two vibrational modes. A low-frequency vibrational mode strongly depends on pressure and is almost independent of temperature, while a high-frequency mode is relevant to the pressure-independent heat motion of molecules. The geometric criterion of hydrogen bonds has been used to evaluate their continuous lifetime as depending on temperature for molecules with different coordination values. The average lifetime of a hydrogen bond substantially depends on the coordination of molecules, with the temperature dependence of the coordination obeying the activation dynamics.

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